Project H-7: Storage of hydrogen in metal hydrides based on transition metal hydrogen complexes

D. Noréus *IEA HIA 2003 AR*
Stockholms University, Stockholm, SWEDEN
E-mail: dag@struc.su.se

Malin Mårtensson et al. showed in ab initio quantum chemical calculations that the bonding between the central transition metal and hydrogen predominately involves only s-d orbitals in the transition metal hydrido complexes, which are the basic building units of this type of hydrides. The 3d-orbitals are less diffuse in character than the d-orbitals in the later rows. This makes the direct bonding between the first row transition metal (TM) and hydrogen more difficult for the corresponding 3d transition metal hydrido (TMH) complexes, than for the later TMs. This is also reflected in the significantly larger variety of TMH complexes found for the later transition metals.

To support the bonding with the first row transition metal, the counter ions have to make a significant contribution. Magnesium is very suitable for this, as it is small and polarizing. In Mg_2NiH_4 magnesium-hydrogen interaction is essential for the stability of the NiH_4 complex. In all other quarternary hydrides containing this NiH_4 complex found so far, magnesium counter ions have been present.

Our work has focussed on trying to understand how important the counter ions are for the stability of TMH-complexes of the first row TMs, and to find ways to weaken this bond in order to make the systems more unstable and better suited for reversible hydrogen storage at low temperatures. This has been done by doping the Mg_2NiH_4 system with impurities and also to try to disturb the lattice by different types of disorder. We have also been engaged in attempts to find new TMH-complexes from the first row of TMs with magnesium counter ions. Later we want to try to destabilize them in a similar manner as for the Mg_2NiH_4 system. This work is still ongoing, but preliminary results have been presented in our list of publications.

M. Olofsson-Mårtensson, U. Häussermann, J. Tomkinson, D. Noréus: “Stabilization of Electron-Dense Palladium-Hydrido Complexes in Solid State Hydrides”, J. Am. Chem. Soc., **122** (2000) 6960-6970